1-Eicosanol

629-96-9 | DTXSID0027272

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.50e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.47e-01

Confidence level: 7.55e-01

Nearest Neighbors from the Training Set

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Terbuthylazine
Measured: 1.10e-11
Predicted: 1.23e-11

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Simazine
Measured: 1.10e-11
Predicted: 1.22e-11

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2-(2-Butoxyethoxy)ethanol
Measured: 7.44e-11
Predicted: 5.15e-11

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Butane, 1,1'-
[methylenebis(oxy)]bis-
Measured: 3.39e-11
Predicted: 3.22e-11